Report of the Beamline Advisory Team of the BCDI beamline
First BAT meeting, 27th February, 2018

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I. Overview and Scientific Case:

On February 27th, the Beamline Advisory Team (BAT) for the Bragg Coherent Diffraction Imaging (BCDI) beamline at NSLS-II met to review the initial beamline science objectives, design, and alternatives. The brilliant coherent x-ray flux in the 6-15 keV range afforded by the NSLS-II will enable a new generation of nanometer scale strain imaging of materials. The scientific goals of the beamline will be to image and study dislocations, defects, and strain in a variety of materials such as nanocrystals, powders, and single grains in polycrystalline materials. Application areas are to include *in operando* studies of battery materials, chemical reactions on crystalline materials (i.e. catalysis, etc), the effects of electrical and magnetic fields on functional materials, deformation in structural materials, and a multitude of time resolved and pump-probe applications. The initial scope proposed covered the length scales of one to possibly ten micron sized crystals at the few to 100 nm resolution probing dynamics from 100's ps to minutes. Below the BAT reports on the general comments on the presented alternatives for the beamline design. We also address six specific charge areas.

The BAT appreciates the detailed and clear presentations from all speakers. Specific comments are below, however, the overall impression is of a well thought through instrument that addresses timely scientific questions and would be unique in the world. The BCDI leadership and team are to be praised for their efforts thus far.

II. General Comments on Beamline Design:

The undulator options were presented by Oleg Chubar. Small gains over a standard IVU 19 mm device could be obtained by some R&D. BAT considered that these gains were less important than the enormous gains that could be delivered by the optimized optical designs. Multi-micron sized crystals will give relatively strong signals; optimization of the coherent illumination will be more important than raw coherent flux.

A second concern was brought up by BAT concerning the onset of dynamical diffraction in crystals of this large size. Typical Laue extinction lengths at 9keV:

Cu_3Au(111)	3.7μm
Gold(111)	2.1μm
BTO(110)	9.0μm
InP(111)	9.3μm
Si(111)	21μm
La_2CuO_4(103)	8.8μm
$LaSrMnO_4$(110)	8.1μm

Clearly these are in the size range of interest to the BCDI beamline users. While the lengths get longer at higher energy, favoring 15keV, they would be a reason that not all sample sizes might be accessible all the way down to 5keV.

Following BAT discussions, these concerns were dismissed for a couple of reasons:
i) the effect of refraction shows up as a phase, varying slowly from one side of the crystal to the other, which can be corrected
ii) strained crystals are of more interest anyway and these would suffer less from dynamical effects.

Oleg Chubar presented his coherence-propagating modeling of the optical design proposed in the original beamline proposal document. The key feature of that design was a "zoomable" beam size from 1μm to 7μm, increased now to 10μm. The challenge is to keep exactly the full coherent flux in the focal spot on the (fixed) sample and the size is zoomed. This will allow matching to samples of different size. BAT agrees with increasing this specification as a future expansion measure to match the longer detector arm and possible future decrease in pixel size on available detectors.

The original design was zoomable only in the horizontal and assumed the sample would be placed out-of-focus in the vertical. Slit-based zooming was possible because NSLS-II has over 100 coherent modes in the horizontal; the mode to be retained can be cut out at two different locations. Oleg identified a second problem with the slit-based zoom method that using a secondary source aperture (SSA) in the horizontal would introduce Fresnel fringes on the focus and cause significant loss of coherence at the edges. This behavior was aggravated by the short beamline format.

Oleg proposed a new design that replaces the SSA with variable entrance apertures on the KB optics. In the horizontal, zooming is achieved by a bendable front-end focusing mirror that moves the effective source position forward and back; the demagnification of the fixed-focus KB mirror gives a variable spot size; the degree of coherence is then selected by adjusting the size of the entrance slit in the front end. The vertical direction is similar in using a bendable front-end mirror to relocate the source; but here the object distance of the vertical KB mirror has to be changed to bring the image into focus; coherence is varied with the entrance aperture of the vertical KB. The result achieves the goal of providing a fully zoomable spot with the sample at the waist of the focus in both directions.

The calculations support the scheme and show that it can work even with a short format beamline, although the aberrations due to imperfect optics would be worse because of the shorter focal lengths on all four active optical elements. The scheme works even better for a long format beamline with the four optical elements conveniently located in a conventional-sized FOE hutch and the experimental hutch itself.

The new zoom design comes at a significant increase of demands on the hardware capability, in the form of two dynamically bendable mirrors and a movable vertical KB mirror which moves by 1m along the beam to cover the full zoom range. To maintain the focus at the center of the diffractometer, with fixed figure mirrors, we expect that two axes of motion on the vertical mirror will be required. There is a slight saving of not requiring a special hutch to hold the SSA. We were informed that all mirrors were within the size range where good quality can be expected and do not push the limits of manufacturing. BAT was happy with the chosen optical design and was impressed with the quality of the simulation results. We discussed the question of ease of alignment of such a complicated optical design and considered that this was manageable: the KBs would be placed in their calculated positions, then the FOE mirrors would be individually bent and steered to maximize flux, and finally the coherence would be set by closing the single aperture that controls it. The current DOE hard x-ray wavefront sensing program will likely provide benefit for the optimization of optics. The BAT recommends that NSLS-II and the CDI beamline investigate ways to tap into the DOE wavefront sensing program.

The only potential drawback of the proposed optical concept implemented in a long beamline is the potential for movement (vibration and/or drift) between the upstream optics, which would reside on the storage ring floor, and the focusing optics, which would reside on a separate floor in an outbuilding. The risk here is that the beam delivered to the focusing optics deviates from the ideal optical axis (for those focusing optics). This can readily be mitigated by the focusing optics having an aperture that is sufficiently large to account for any vibrations, while it is expected that active feedback will correct for drifts. It is unlikely that such an aperture increase is at all significant for the optics design, nevertheless, it would be best practice to model explicitly this case and conclude on the optimal design for the focusing mirrors aperture and height error based on such a study.

III. BAT Response to NSLS-II Charge

BAT discussed the six charges presented by John Hill and has come up with the following responses.

1. Science Case for Time-Resolved Program:

> Charge: "The viability of elements of the science case to be undertaken at the state-of-the-art in light of the NSLS-II source properties. In particular, one component of

> the science case is the pump-probe, time-resolved capability. Please comment on the strength of this science case in light of the current and future properties of the NSLS-II source."

The proposed BCDI beamline is complementary to all other beamlines of its kind worldwide. However, it has a unique sample size range that is not duplicated elsewhere. The time-resolved capability would be a planned future upgrade, not implemented on day 1. But the science case for laser driven pump-probe experiments on multi-micron sized crystals is compelling. Vibration periods of such crystals will be in the hundreds of picosecond time range and the expected pulse length of single 10mA bunches was shown to be under 50ps at NSLS-II.

The presentation of Gabriele Bassi showed the "camshaft" mode of NSLS-II could provide approx. 100 ps duration pulses with a reasonable fraction of the ring current (10 mA) within a single pulse. It is expected that the commensurate photon flux, combined with the very high scattering cross section of the scientifically relevant crystals, is more than sufficient to support the case for time-resolved experiments at the BCDI beamline of NSLS-II. Nevertheless, to further support this aspect of the science case, the development team should specify coherent x-ray fluxes expected at the sample for various timing modes of the NSLS-II bunch structure. Unless this time structure is found to be incompatible with other conflicting directions of NSLS-II, there will be a rich field of imaging transient strain patterns in such samples. The capability for 100 ps time-resolved science will quite likely disappear at APS and other sources when they upgrade to MBA lattices. The hundred picosecond time range is difficult to justify at XFELs, which appear to favor femtosecond and single picosecond experiments, and would never have the capacity to complete with BCDI at NSLS-II. Furthermore, no existing or planned XFEL instrument has the capability to explore the detector angular range addressed by the BCDI beamline, nor the two-arm capability which is unique in both the synchrotron and XFEL worlds.

The options to provide laser hutches and hardware like event receivers in the baseline BCDI plan is a relatively low cost and would greatly facilitate installation of the lasers when these are funded. BAT recommends this be included in the plan. The required hutch penetrations, and the routing to the interaction region should all be planned and installed in the first phase of the project too, as these are of relatively low cost and effort in the installation phase and would cost both more resources, effort and downtime once the beamline is operating.

Overall, the time-resolved case is strongly supported as a unique and feasible capability. The BAT sees it important that this capability remain in the long-term planning for BCDI, even if it is not available for day 1 operations.

2. Technical Requirements:

> Charge: "The technical requirements and characteristics of the presented beamline and endstation concepts; are they consistent with upholding the described science case?"

In general, the BAT felt that the technical requirements strongly upheld the scientific case for the BCDI beamline. The available coherent flux, novel two arm detector system, and large delta scan range will make it a unique facility. It would be desirable to have a larger range of detector motion out-of-plane as this gives a wider range of Bragg peaks accessible for a given sample. However, this is offset by the idea of providing a full 3-axis goniometer on the sample stage. The sample stage can be improved by including a vertical precision air-bearing stage underneath a kappa-phi combination. The development team should continue to investigate precision alternatives to an off-the-shelf kappa stack. In principle, a ninety degree arc on top of a full rotation air-bearing with another phi circle inside of the ninety degree arc could have better performance. An XYZ piezo stage and conventional wide range XYZ directly underneath the sample with a load capacity of 1kg will cover a wide range of sample options.

The proposed 2-arm option for the detectors is attractive as it would enable the simultaneous examination of 2 neighboring crystals within the same sample to investigate their interactions when the sample undergoes *in-situ* environmental changes. However, this would require simultaneous optimization of the diffraction conditions of two crystals on one goniometer. The development team should seriously investigate the possibility of actually doing this on a sample of interest such as polycrystalline metals.

It would be good to provide a capability for locating and orienting grains within a polycrystalline sample. It was discussed whether this can be achieved with the planned BCDI detector system and Double Multilayer Monochromator (DMM), perhaps by rastering the energy or diffraction tomography. BAT recommends these options be investigated.

A clearance of 0.4 m is proposed between the sample and the incident beam delivery optics, which is good for allowing a Kappa diffractometer to swing freely and enables a wide range of alternative sample environments. However, the radius of the proposed goniometer was not specified. What is the current thinking for the actual dimensions of the experimental apparatus that will be installed on the goniometer? This optical working distance also allows placement space for future laser delivery optics. BAT suggests this would be a good closest approach distance for the detector arm(s) also. A 0.4 m detector distance would facilitate the near field diffraction capability mentioned above. 1.0 m is currently proposed. An appraisal of the feasibility of a 0.4 m minimum detector to sample distance is requested.

3. Pros and Cons of Current Design:

> Charge: "The pros and cons of the different presented design concepts. In addition to their viability in upholding the described science case, are they technically feasible? Please comment on the length of the beamline, the size of the experimental hutch, detector options, infrastructure provisions, and choice of insertion device."

BAT members were initially interested in the possibility of a "gantry" detector positioning system, similar to that at the PDF beamline at 28ID. But after seeing the difficulty of scaling such a structure to 8 m radius, BAT decided in favor of the proposed raised arc structure. BAT noted that NSLS-II already has experience building such a structure and that the added weight may help with stabilizing the external building.

The 90° horizontal detector geometry would see very weak signals because of polarization effects. These can be mitigated with a transmission diamond phase plate inserted in the incident beam to rotate the polarization. The phase plate would also enable studies of magnetic contrast in samples with circularly polarized x-ray beams.

BAT raised a serious issue of lack of temporal coherence to coherently illuminate multi-micron sized crystals with a Si(111) Double Crystal Monochromator (DCM), even with a vertical axis (which BAT favors). This would be alleviated by providing a Si(311) DCM as an alternative. The development team should seriously investigate the limitations of temporal coherence and the impact on every aspect of the instrument design. It might be that even with Si(311) crystals in the DCM there is not sufficient coherence to study high order Bragg peaks from larger samples. So the benefits of the larger angular range of the detector arm may only apply to smaller samples and possibly be less important. For example, at 9 keV a Silicon (333) monochromator would have about 8 micrometers of longitudinal coherence, enabling 120 degree diffraction from samples in the 5 micrometer scale since one needs the beams reflected from both the front and back of the sample to coherently interfere.

BAT recommends 4-sigma or greater sizing of the mirrors, so that alignment will be facilitated and the edge effects of manufacture will be avoided. For the current design, these are not expected to be particularly expensive. The APS mechanical bender, currently under development, was mentioned as a possible solution for the first mirror pair of the beamline.

On the choice between a long and a short format of the beamline, BAT had a clear preference for the long, 100m design. Among the reasons are:

i) the optical design is more favorable, although the full simulation is still not complete.

ii) based on numbers presented for 3ID, the vibrations would be significantly reduced and the correlation length of any remaining vibrations is longer than the sample-to-focusing optic distance.

iii) the layout at sector 9ID looks particularly favorable, as the 8 m detector arm fits comfortably and there are fewest sources of external interference.
iv) the possibility of a longer build schedule is not a constraint because there is no budget-induced urgency to complete the beamline quickly.

4. The future upgrade potential and associated tradeoffs:

Charge: "The future upgrade potential and associated tradeoffs in the beamline design. E.g. wide bandpass optics for higher flux for a certain range of science applications."

The upgrade to a full laser pump-probe system is attractive and strongly supported by BAT. It is suggested to already engage with the user community and specify the laser system soon, despite the relevant funding not yet being secured apparently. This will ensure adequate specification of the laser hutch, as well as a relatively rapid deployment should funding be found.

The DMM is advantageous for the white-beam Laue diffraction capability and may allow very fast polychromatic imaging that would work well for laser pump-probe experiments. Its inclusion in the scope is supported by BAT.

5. Cost and schedule estimates:

Charge: "Are the estimates presented realistic for this stage in the development of the beamline design?"

BAT thought these looked reasonable at first appraisal. While it would be desirable if the beamline could be delivered before the expected APS shutdown, such a schedule goal should not compromise the capability of the BCDI beamline. It will be unique in the world and is better delivered at ideal specification later, rather than with compromised specification earlier, in order to allow optimal exploitation of its unique capabilities.

6. Potential risks, technical or otherwise:

Charge: "Please comment on potential risks, technical or otherwise, associated with the presented concepts, including potential ESH concerns."

Below we summarize the BAT's comments and concerns for potential risks:

- The 16m long air bearing track for the detector looks challenging and a preliminary engineering design and risk analysis would be appreciated. Nevertheless, it seems a superior design to the gantry alternative presented.
- Additional human resources will be needed in 2018 to deliver the final design review (FDR) on the planned time scale. In particular, the engineering and other design resources that will be necessary to properly specify the

instrument are essential to be available from conceptual design review (CDR) through FDR and procurement.

- The 9ID location appears to be the least risky choice with superior vibrational properties, least external interference, and the greatest flexibility for optimal X-ray optical design.
- The gantry option for the detector positioning would introduce a big risk of collisions and/or cost to develop an intelligent collision avoidance system. It may also have EHS ramifications due to the suspended nature of the detectors and its large scale. It would also require very complex controls to perform its function, which would cost both resources and introduce risk. For all these reasons, the "two-arm" design is greatly preferred over the gantry design.
- The kappa-geometry sample goniometer might be risky from the stability requirements. BAT notes that the bad sphere-of-confusion axes (kappa and phi) would not be moved during a measurement, while the vertical precision air-bearing stage (micron sphere-of-confusion) would be used for most 3D scanning.
- Algorithm development is urgently needed to take full advantage of the ability to invert diffraction from strong phase objects represented in real-world materials, as many of the planned applications will involve.
- The multimodal imaging capabilities of BCDI would be greatly helped by the introduction of NSLS-II standards for sample mounts.
- If the zoom optics system does not work, what is the plan? Will the system be designed such that the smallest spot size is the default spot if mirrors are just surveyed into place and left static? How would this choice impact the science program? This is particularly concerning when considering the long beamline option. The raw, unfocussed beam, will have relatively long coherence lengths. Therefore, extremely poor flux density. What would be the achieved spot size if the first mirrors were left flat and the planned figured KB were the only focusing elements in the beamline?
- The best achieved temporal coherence from the DCM may indeed limit the range of samples that can be studied. How does this impact the proposed science case?
- The undulator choice does not appear to be a risk.
- Detector choices will need careful evaluation.
- Sample laboratories for users should be co-located with the experiment hutch—ideally adjacent to the hutch. A clean area is also required, such as a clean tent, a flow box, or ideally both as they can serve different functions. A complete clean room is not likely to be required. The cleanliness plan for the experiment station, in particular the sample region, should be outlined at least at the conceptual level in the beamline's CDR.